Pore-Level Modeling of Carbon Dioxide Sequestration in Deep Aquifers

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ABSTRACT

Underground injection of gas is a common practice in the oil and gas industry. Injection into deep brine-saturated formations is a commercially proven method of sequestering CO_2. However, it has long been known that the immiscible displacement of a connate fluid by a less-dense and less-viscous fluid produces gravity override and unstable displacement fronts. These phenomena allow only a small fraction of the pore volume of a brine-saturated formation to be available for sequestration. A better understanding of the fluid displacement process could lead to reduced capital and operating costs by increasing CO_2 sequestration in deep aquifers.

We have developed a pore-level model of the immiscible injection of a non-wetting fluid (CO_2) into a porous medium saturated with a wetting fluid (brine). This model incorporates a distribution of different "pore-throat" radii, the wettability of the formation (i.e., the gas-liquid-solid contact angle), the interfacial tension between the fluids, the fluid viscosities and densities, and all other parameters that appear in the capillary pressure or the capillary, Bond, or fluid-trapping numbers. The computer code for the model maintains a constant injection velocity to within a few percent.

This model has been used, with experimental values of viscosities and interfacial tensions, to study the high-pressure injection of carbon dioxide into brine-saturated porous media. Results are presented for the applied pressures, fluid-front geometries, residual saturations, and numbers of blocked throats.

INTRODUCTION

The possible effects of rising atmospheric concentrations of carbon dioxide on global climate are of worldwide concern. The U. S. Department of Energy and its National Energy Technology Laboratory have instituted programs to study various methods of sequestering CO_2.[1], [2] Underground injection of gas has long been a common practice in the oil and gas industry.[3] Injection into deep brine-saturated formations is a commercially proven method of sequestering CO_2.[4] However, it has long been known that the immiscible displacement of a connate fluid by a less-dense and less-viscous fluid produces gravity override and unstable displacement fronts.[5] These phenomena allow only a small fraction of the pore volume of a brine-saturated formation to be available for sequestration.[6] A better understanding of the fluid displacement process could lead to new technologies for alleviating these mobility control problems[5] and to reduced capital and operating costs for CO_2 sequestration in deep aquifers.

We have developed a pore-level model of the immiscible injection of a non-wetting fluid (CO_2) into a porous medium saturated with a wetting fluid (brine).[7] This model, which is an extension of an earlier model for two miscible fluids,[8] incorporates a distribution of different "pore-throat" radii, the wettability of the formation (i.e., the gas-liquid-solid contact angle), the interfacial tension between the fluids, the fluid viscosities and densities, and all other parameters that appear in the capillary pressure or the capillary, Bond, or fluid-trapping numbers. This model has been used, with experimental values of viscosities[9] and interfacial tensions,[10] to study the high-pressure injection of carbon dioxide into brine-saturated porous media. Results are presented for a variety of capillary numbers, showing trends in the applied pressures, fluid-front geometries, and residual saturations.

DESCRIPTION OF THE MODEL

This pore-level model of injection of carbon dioxide into a water-wet porous medium incorporates, as realistically as possible, both the capillary pressure blocking the invasion of narrow throats and the viscous pressure drop in a flowing fluid. The two-dimensional model consists of a square lattice of pore bodies with unit volume at the lattice sites and connecting throats, which are of unit length and have randomly chosen cross-sectional areas between 0 and 1. We choose to inject the carbon dioxide along a diagonal; if we had chosen to inject along one side of the square lattice, we would have the artificial situation of one-half of the throats perpendicular to the average pressure gradient, making them more susceptible to capillary blocking because of a reduced pressure drop. This model is similar in spirit to other recent modeling efforts; but our model has some features which should make it more physical than other models: e.g. pore throats with real volumes, pore bodies with finite volume, constant velocity (giving a meaningful capillary number), and multiple checks on whether pores are blocked or unblocked.[11],[12],[13]

When the interface is in one of the pore throats, the radius of curvature, R, of the meniscus is fixed by contact angle, θ, and the radius of the pore throat, r ;

$$R = r / \cos\theta. \tag{1}$$

Therefore, the pressure drop across the meniscus is fixed at the capillary pressure

$$P_{cap}(R) = \frac{2\,\sigma\cos\theta}{r}, \tag{2}$$

where σ is the surface tension. Thus the flow velocity is given by the throat conductance times the total pressure drop across the throat, see Fig. (1a).

$$q = g_{throat}\,(P_{nw} - P_w - P_{cap}). \tag{3a}$$

Here, pressure P_{nw} is the pressure in the non-wetting, CO_2 -filled pore body, and P_w is the pressure in the wetting water-filled pore body. The transmissibility (conductance) of the throat is given by Poiseuille's law [14]

$$g_{throat} = \frac{1}{8\pi\mu_w}\;\frac{A_{throat}^2}{(x + (1-x)/M)} \tag{3b}$$

where μ_w is the viscosity of water, A_{throat} is the cross-sectional area of the throat, (randomly chosen from a uniform distribution between 0 and 1), x is the fraction of the throat of length 1 which is water-filled, and M is the ratio of the water viscosity to that of the carbon dioxide. From Eq. (3a), the CO_2 advances if the pressure difference between the CO_2 -filled pore and the water-filled pore exceeds the capillary pressure. Otherwise the CO_2 will retreat.

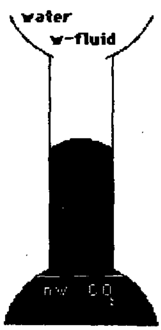


Fig. 1a
Meniscus in throat

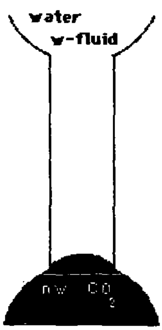


Fig. 1b
Meniscus at inlet

Blocking is possible in 1.b (see Eq. (5))

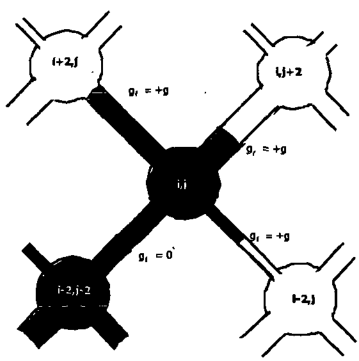


Fig. 2
Example for determining gf in Eq. (6).

If the interface is at the entrance to a throat Fig. (1b)), the throat will be blocked if the pressure difference is positive but not large enough to overcome the capillary pressure in Eq. (2). In this case, the positive pressure difference creates a meniscus with a radius of curvature, R, satisfying the equation

$$P_{cap}(R) = \frac{2\,\sigma\cos\theta}{R} = P_{nw} - P_w, \tag{4}$$

where this radius of curvature is larger than the radius R in Eq. (1) needed to enter the throat. Therefore the throat is blocked (q = 0) whenever a positive pressure drop is too small to push the meniscus into the throat, i.e. , whenever

$$0 < P_{nw} - P_w < \frac{2\,\sigma\cos\theta}{r}. \tag{5}$$

If the pressure drop in Eq. (5) is negative (q is negative ; $q = g_{throat}(P_{nw} - P_w)$), the water re-invades the pore body ; and if the pressure drop exceeds the capillary pressure, the non-wetting fluid advances; q is positive and given by Eq. 3a.

Volume conservation of the incompressible fluid dictates that the net volume flow, q, out of any pore body must be zero. Using the above rules for the flow velocities, requiring that the net flow out of pore body (i,j) be zero leads to the following equation for $P_{i,j}$:

$$
\begin{aligned}
(g_{i-2,j-1} + g_{i,j+1} + g_{i-1,j} + g_{i+1,j})P_{i,j} = \quad & \quad (6)\\
(g_{i-2,j-1} P_{i-2,j-2} + g_{i,j+1} P_{i+2,j+2} + g_{i-1,j} P_{i-2,j} + g_{i+1,j} P_{i+2,j}) + &\\
(gf_{i-2,j-1} P_{cap,i-2,j-1} + gf_{i,j+1} P_{cap,i,j+1} + gf_{i-1,j} P_{cap,i-1,j} + gf_{i+1,j} P_{cap,i+1,j}) &
\end{aligned}
$$

Here the array gf is zero if there is no meniscus in the throat; for a meniscus in the throat gf = +g or -g depending on the direction of CO_2 advance in the throat (Fig. 2).

To determine the pressure field one iterates (Eq. 6) until stability is achieved (the residual is less than some small value); i.e. until

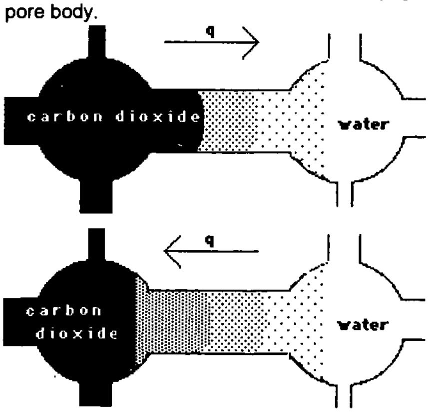
$$R = \sum (P_{new} - P_{old})^2 < \varepsilon , \qquad (7)$$

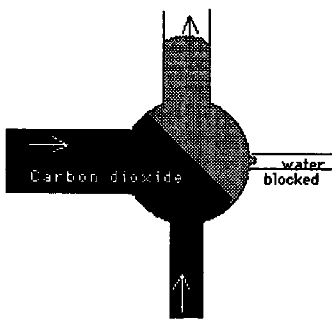
where ε is chosen to be small (e.g. $10^{-6} > \varepsilon > 10^{-9}$). This value of ε was adjusted to minimize run-time without seriously sacrificing mass-conservation.

At a given time step, once the pressure field is determined for the initial choice of conductances, the interface is scanned to determine if there are changes in the throat blockages because of changes in the pressure drops. With these new conductances, the pressure field is redetermined by iterating Eq. (6). With the new pressure field, changes,in the blockages are re-determined. This procedure continues until there are no further changes in the blockages, or until the changes occur only in throats that have alternated (blocked to unblocked) three times or more.

Once the pressure field has been determined and there are no more changes in throat blockage (excluding the oscillating blockages discussed above), we know the pressure field that will advance the interface. We choose a time interval that will advance the fluid one-half unit volume through the throat with the largest flow velocity.

Flow can increase the amount of non-wetting fluid (CO_2) within the pore throat, or through the pore throat into the pore body (Fig. 3a). Similarly, backflow can cause the interface to retreat within the pore throat (Fig. 3b) or through the pore throat into the pore body.





Flow Rules: Fig. 3a) Top ; 3b) Bottom

Fig. 3a) flow can advance the interface through the throat into the pore body

Fig. 3b) the interface can retreat from a pore body into the throat and into the next pore body

Fig. 4 If the flow over-fills a pore body at a given step, the over-filling is shared by the unblocked throats

If the pore body becomes over-filled by carbon dioxide, the excess fluid is shared proportionally by the outflow throats (Fig. 4). However, if at these pressures the carbon dioxide is blocked from entering any throats, the last time interval is recalculated so that the fluid will just fill the pore body with an excess of 5% or less. Similarly, if the water backflow fully re-invades a pore body, the excess water is shared by the outflow throats.

If the carbon dioxide occupies two adjacent pores, without fully occupying the throat between them, there is a trapped plug of water in the throat. This plug will remain trapped in the throat unless the pressure drop across the throat is large enough to mobilize the plug of wetting fluid. The pressure drop across the throat must be larger than the capillary pressure to push the water out of the throat. If the pressure drop is large enough, we allow this water to reside in the pore until such a time as that pore is fully re-invaded by water. This assumption that the water remains in the pore is unphysical, because it is more favorable to have the wetting fluid re-invade the narrower throats filled with non-wetting fluid. The fraction of wetting fluid (water) participating in this unphysical process is calculated in the program. On the other hand, if water re-invades two adjacent pore bodies, without re-invading the connecting throat, the non-wetting carbon dioxide is moved to the low-pressure pore body.

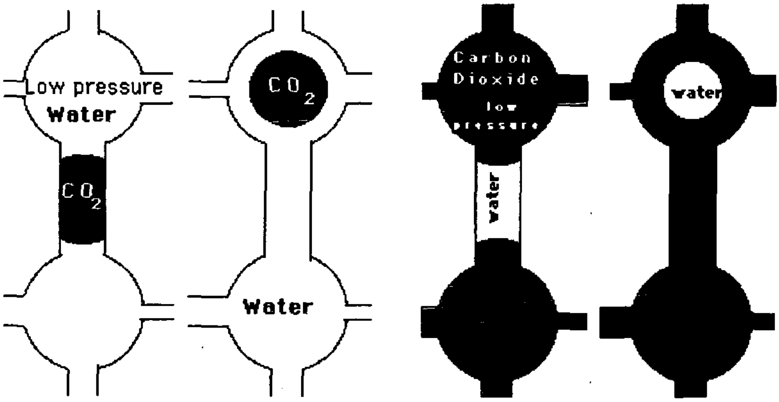


Fig 5a) Trapped CO_2 will be moved to the lower pressure pore body.

Fig. 5b) Trapped water will be moved to the low pressure pore body for a pressure drop exceeding the capillary pressure

A throat is considered to be on the interface, if the pore body at one end contains some water and if the pore body at the other end is fully invaded by carbon dioxide (or was fully invaded and is not yet fully re-invaded by water due to backflow).

RESULTS

We have chosen parameters appropriate to high-pressure injection of carbon dioxide injection into a typical brine saturated reservoir: an interfacial tension, $\sigma = 21\frac{\text{dynes}}{\text{cm}}$, a contact angle of $\theta = 0^{\circ}$, and a viscosity of the high pressure CO_2 , $\mu = 0.05$ cp.[9,10,15]

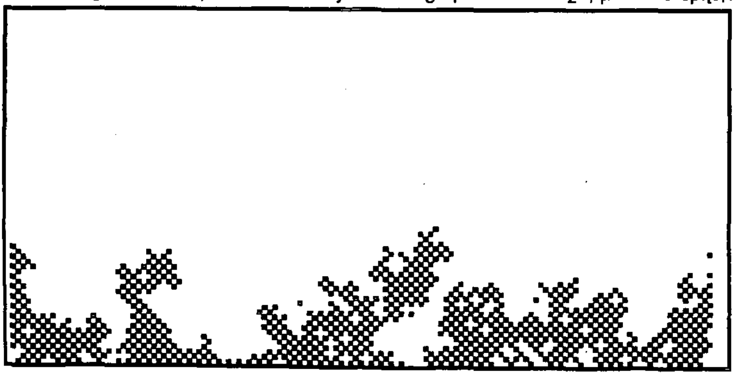


Figure 6) The flow pattern, the black pores are occupied by carbon dioxide.

We chose the scale of the medium (length of a typical throat) to be $\ell = 100$ μm; thus, in our model porous medium, the largest throats will have a radius of 56 μm, and the smallest capillary pressure (in this largest throat) will be $P_{cap,min} = 7500\ \frac{\text{dyne}}{\text{cm}^2}$. Using these values of the parameters, we have run this program on a 70x70 square lattice array, adjusting the pressure drop, ΔP, to maintain a constant flow velocity $q = \frac{q^*\ \ell^3}{8\pi\ \text{sec}}$ with $q^* = 116.0 \pm 1.4$. For these parameters the capillary number is 3×10^{-5}. Figure 6 shows the flow pattern after 10,000 time steps. The black areas are invaded by carbon dioxide. At this time the saturation is 24%.

As mentioned, the velocity is approximately constant; small variations are within a standard deviation of less than 2%. To maintain this constant velocity, the pressure drop shows wide variations (see Fig. 7).

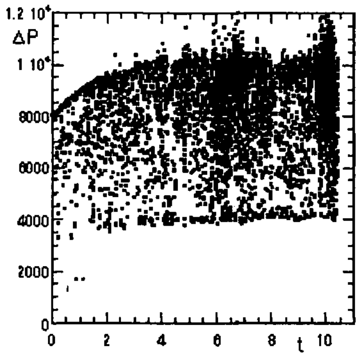


Figure 7) Pressure drop across the porous medium as a function of injection time.

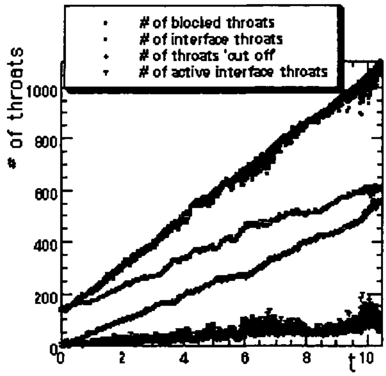


Figure 8) Number of throats of different types as a function of injection time.

Figure 8 shows the dramatic effect of capillary blocking of the throats, near the end of this simulation there are 600 throats on the interface. Of these 600 throats, only 90 are active with the rest being blocked. The total number of blocked throats consists of the 510 interfacial throats that are blocked and the 560 throats that have trapped, immobilized water (as in Fig. 5b, with the pressure drop being too small to mobilize the trapped water).

Additional computer runs will lead to a greater understanding of the role of capillary trapping in CO_2 sequestration and of the effectiveness of different sequestration schemes.

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